Numerically Consistent Equations for the Function v = v(p,T)in an Extended Critical Region of Water

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Usually equations of state are set up as Helmholtz-functions f = f(T,v), from which all other thermodynamic properties can be derived analytically. If any thermodynamic property is to be calculated for pressure p and temperature T, the specific volume v has to be calculated iteratively from p = p(T,v) before. Initial values needed for this iteration are calculated from auxiliary equations v = v(p,T). For the liquid and the gas regions of water very precise auxiliary equations are available and can be set up for other fluids by use of advanced approximation methods. But setting up such equations for the critical and supercritical region is more complicated.

The paper presents equations v = v(p,T) for water for an extended critical region in the range of temperature between 615 K and 900 K and pressure up to 100 MPa. This region had to be split into subregions because of the nonanalytic behavior of v = v(p,T) when crossing the phase boundary and in order to achieve a good consistency to the basic equation p = p(T,v). Along the subregion boundaries the equations fit together extremely close; owing to this there shouldn't result problems from the division into subregions. Furthermore, the equations are extremely consistent to the basic equation p = p(T,v), i.e. they are numerically consistent. Therefore in many cases no iteration is necessary when using the equations presented. For setting up the structure of the equations an algorithm derived from the structure optimization method by *Setzmann* and *Wagner* was used. The coefficients of the equations were determined using the least squares method in combination with an iterative weighting algorithm being aspired to minimize the maximum (normalized) deviation between the auxiliary and the basic equations. The terms fed to the structure optimization algorithm were developed considering the infinite slope of the specific volume at the critical point as well as the need to set up equations with low computing time consumption, i.e. equations with no or only few transcendental functions.